Expansions in series of varying Laguerre polynomials and some applications to molecular potentials

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Abstract

The expansion of a large class of functions in series of linearly varying Laguerre polynomials, i.e., Laguerre polynomials whose parameters are linear functions of the degree, is found by means of the hypergeometric functions approach. This expansion formula is then used to obtain the Brown–Carlitz generating function (which gives a characterization of the exponential function) and the connection formula for these polynomials. Finally, these results are employed to connect the bound states of the quantum–mechanical potentials of Morse and Pöschl–Teller, which are frequently used to describe molecular systems.

Keywords: Varying orthogonal polynomials; Laguerre polynomials; Connection problems; Generalized hypergeometric functions; Morse potential; Pöschl–Teller potential

1. Introduction

Let $\{\omega_n(x)\}$ be a sequence of weights on $\Delta \in \mathbb{R}$, and $p_{n,m}(x)$ denote the mth polynomial orthogonal with respect to $\omega_n(x)$,

$$\int_{\Delta} p_{n,i}(x)\, p_{n,j}(x)\omega_n(x)\, \mathrm{d}x = h_{n,i}\delta_{i,j}.$$

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In recent years, much attention has been paid to the study of the asymptotic behaviour and the distribution of zeros of the sequence of polynomials $\{p_{n,n}(x)\}$, which are called *orthogonal polynomials with varying weights* [3,4,6,7,9,12,18,29]. These polynomials are interesting not only because of their own mathematical properties, but also due to their numerous applications in matrix theory, numerical analysis, and classical and quantum physics. Indeed, (a) they have been used to prove universality for various spectral statistical quantities arising in random matrix models [9], (b) they play a relevant role in the theory of convergent sequences of interpolatory integration rules [3], as well as in the study of Hermite–Padé approximants [7], (c) they have been shown to represent spectral functions of turbulence fields [28], and (d) they are often encountered in the wavefunctions of some quantum–mechanical potentials modelling a wide variety of physical systems [2].

Here we deal with the expansion problem for varying orthogonal polynomials, which, up to our knowledge, has not yet been considered in the literature. We confine ourselves to the expansion problem for Laguerre orthogonal polynomials with linearly varying weights; i.e., the problem of finding the coefficients in the expansion

$$f(x)=\sum_{n=0}^{\infty}c_nL_n^{(an+\alpha)}(x), \tag{1}$$

where $f(x)$ is an arbitrary function and the varying Laguerre polynomials $L_n^{(an+\alpha)}(x)$ are orthogonal with respect to $\omega_n(x)=x^{an+\alpha}\,\mathrm{e}^{-x}$. The polynomials $L_n^{(an+\alpha)}(x)$ with $a=-2$, which are closely related to the Bessel polynomials [13,14], appear in the wavefunctions of the Morse potential (see Section 4) and have also found application in problems of classical physics [28]. The polynomials $L_n^{(an+\alpha)}(x)$ with $a=-1$ were considered as early as 1952–53 by Toscano [30] and Shively [27]. The latter author pointed out that these polynomials have a generating function of exponential type, so that they are of Sheffer A-type zero (see, e.g., [22, Chapter 13]), and this property was later shown to hold for arbitrary complex values of a [5,8]. More recently, the asymptotic behaviour of the polynomials orthogonal with respect to the more general weights $\omega_n(x)=x^{\alpha_n}\exp(-\beta_n x)$, where $\alpha_n=\alpha n+\mathrm{o}(n)$, $\beta_n=\beta n+\mathrm{o}(n)$ $(\alpha,\beta>0)$ has been intensively studied [4,6,18,29].

To solve the expansion problem (1), we shall use the hypergeometric functions method, which has been already employed for the corresponding problem involving classical orthogonal polynomials with nonvarying weights [10,11,15,17,23,25]. This is briefly outlined in Section 2, where the well-known connection formula for the standard Laguerre polynomials is obtained. In Section 3, a theorem of Verma [31] is used to determine expansions of hypergeometric functions in series of the varying Laguerre polynomials $\{L_n^{(an+\alpha)}(x)\}$. As a by-product, the poorly known exponential generating function of Brown and Carlitz [5,8] is obtained; moreover, we solve the connection problem between Laguerre polynomials whose parameters are linear functions of the degree. Problems of this kind are very often encountered in the study of the relationships between the wavefunctions of some quantum–mechanical potentials employed for describing physical and chemical properties in atomic and molecular systems. As an illustration, in Section 4 we give explicit relationships among the wavefunctions of the Morse and Pöschl–Teller potentials. Finally, in Section 5, some concluding remarks and a few open problems are given.

2. The hypergeometric functions approach to series expansions for classical orthogonal polynomials

The expansion of a general function $f(x)$ in series of a given system of classical orthogonal polynomials $\{p_n(x)\}$ with nonvarying weights is a long-standing and well-known problem in the theory of special functions. If the polynomial sequence $\{p_n(x)\}$ is orthogonal on an interval $\Delta \in \mathbb{R}$ with respect to the weight function $\omega(x)$,

$$\int_{\Delta} p_n(x)\, p_m(x) \omega(x)\, \mathrm{d}x = h_n \delta_{n,m},$$

and $f(x)$ admits an expansion of the form

$$f(x) = \sum_{n=0}^{\infty} c_n\, p_n(x),$$

every Fourier coefficient c_n can be computed as

$$c_n = \frac{1}{h_n} \int_{\Delta} f(x)\, p_n(x) \omega(x)\, \mathrm{d}x,$$

provided that the integral in the right-hand side does exist and the resulting series satisfies the appropriate convergence conditions (see, e.g., the detailed discussion of the Jacobi case in [17, Chapter 8]). Other characterizations of the polynomials $\{p_n(x)\}$, such as their generating functions or recurrence relations, can also be used to compute the expansion coefficients.

When $f(x)$ and $p_n(x)$ can both be expressed in terms of the generalized hypergeometric function, closed analytical expressions for the expansion coefficients can often be found by taking advantage of known theorems from the theory of generalized hypergeometric functions. For instance, the following theorem of Fields and Wimp [11] (see also [10, 17, Vol. II, p. 7] for more general results of the same kind),

$$\begin{aligned} {}_{p+r}F_{q+s}\left(\left. \begin{array}{c} [a_p], [c_r] \\ [b_q], [d_s] \end{array} \right| zx \right) = \sum_{n=0}^{\infty} \frac{[a_p]_n (\lambda)_n (-z)^n}{[b_q]_n n!} \\ \times {}_{p+1}F_q \left(\left. \begin{array}{c} [n+a_p], n+\lambda \\ [n+b_q] \end{array} \right| z \right) {}_{r+1}F_{s+1} \left(\left. \begin{array}{c} -n, [c_r] \\ \lambda, [d_s] \end{array} \right| x \right), \end{aligned} \tag{2}$$

when used together with the hypergeometric representation of Laguerre polynomials,

$$L_n^{(\alpha)}(x) = \frac{(\alpha+1)_n}{n!}\, {}_1F_1 \left(\left. \begin{array}{c} -n \\ \alpha+1 \end{array} \right| x \right), \tag{3}$$

leads to the general expansion formula [11]

$${}_pF_q \left(\left. \begin{array}{c} [a_p] \\ [b_q] \end{array} \right| zx \right) = \sum_{n=0}^{\infty} \frac{[a_p]_n (-z)^n}{[b_q]_n}\, {}_{p+1}F_q \left(\left. \begin{array}{c} [n+a_p], n+\alpha+1 \\ [n+b_q] \end{array} \right| z \right) L_n^{(\alpha)}(x). \tag{4}$$

As first pointed out by Lewanowicz [15], Eq. (4) includes as a particular case the well-known connection formula for Laguerre polynomials (see, e.g., the proofs in [1, Section 7.1, 22, p. 209, 24]),

$$L_m^{(\beta)}(x) = \sum_{n=0}^{m} \frac{(\beta-\alpha)_{m-n}}{(m-n)!} L_n^{(\alpha)}(x). \tag{5}$$

We recall that the definition of the generalized hypergeometric function is

$${}_pF_q\left(\left.\begin{array}{c}[a_p]\\ [b_q]\end{array}\right| x\right) = \sum_{k=0}^{\infty} \frac{[a_p]_k x^k}{[b_q]_k k!},$$

where $[a_p]$ and $[b_q]$ denote, respectively, sets $\{a_1, a_2, \ldots, a_p\}$ and $\{b_1, b_2, \ldots b_q\}$ of complex parameters such that $-b_j \notin \mathbb{N}_0$, and we use the contracted notation

$$[a_p]_k = \prod_{i=1}^{p} (a_i)_k, \quad [b_q]_k = \prod_{j=1}^{q} (b_j)_k,$$

where $(z)_n = \Gamma(z+n)/\Gamma(z)$ is Pochhammer's symbol. When the series in the right-hand side does not terminate after a finite number of terms, it converges provided that either $p \leqslant q$, or $p = q+1$ and $|x| < 1$. In Eq. (2), the parameters λ, $[c_r]$, $[\beta_u]$, $[d_s]$ and $[\alpha_t]$ are assumed to be independent of n. This formal power series identity holds whenever the series in the left- and right-hand sides are both either terminating or convergent, a remark that also applies to the expansions given in Section 3 below.

3. Expansions in series of varying Laguerre polynomials

3.1. *Expansion of general functions*

We seek for the coefficients in expansion (1), where we assume that the function $f(x)$ can be represented in terms of a hypergeometric series. Let us bring here that according to Eq. (3) the varying Laguerre polynomials $L_n^{(an+\alpha)}(x)$ have the hypergeometric representation

$$L_n^{(an+\alpha)}(x) = \frac{(an+\alpha+1)_n}{n!}\, {}_1F_1\left(\left.\begin{array}{c}-n\\ an+\alpha+1\end{array}\right| x\right). \tag{6}$$

To solve this problem we take advantage of the following expansion formula, first derived by Verma [31]:

$$\begin{aligned}{}_{p+s}F_q\left(\left.\begin{array}{c}[a_p],[b_s]\\ [c_q]\end{array}\right| zx\right) &= h\sum_{n=0}^{\infty} \frac{(h-n\lambda+1)_{n-1}[b_s]_n[e_u]_n(-z)^n}{n![c_q]_n}\\ &\quad \times {}_{s+u+1}F_q\left(\left.\begin{array}{c}[n+b_s],[n+e_u],h+n(1-\lambda)\\ [n+c_q]\end{array}\right| z\right)\\ &\quad \times {}_{p+2}F_{u+2}\left(\left.\begin{array}{c}-n,[a_p],1+h(1-\lambda)^{-1}\\ h-n\lambda+1,[e_u],h(1-\lambda)^{-1}\end{array}\right| x\right).\end{aligned} \tag{7}$$

Taking $p=1$, $[a_p]=h(1-\lambda)^{-1}$, $u=1$, $[e_u]=1+h(1-\lambda)^{-1}$, $q=r+1$, $[c_q]=\{[c_r],h(1-\lambda)^{-1}\}$, (7) simplifies to

$$
{}_sF_r\left(\left.\begin{matrix}[b_s]\\ [c_r]\end{matrix}\right| zx\right)=\sum_{n=0}^{\infty}\frac{(h-n\lambda+1)_n[b_s]_n(-z)^n}{n![c_r]_n}
\times{}_{s+2}F_{r+1}\left(\left.\begin{matrix}[n+b_s],n+1+h(1-\lambda)^{-1},h+n(1-\lambda)\\ n+h(1-\lambda)^{-1},[n+c_r]\end{matrix}\right| z\right)
\times{}_1F_1\left(\left.\begin{matrix}-n\\ h-n\lambda+1\end{matrix}\right| x\right).
$$

Equivalently, writing $\lambda=-a$, $h=\alpha$ and using (6), we have a general expansion formula in series of varying Laguerre polynomials,

$$
{}_sF_r\left(\left.\begin{matrix}[b_s]\\ [c_r]\end{matrix}\right| zx\right)=\sum_{n=0}^{\infty}\frac{[b_s]_n(-z)^n}{[c_r]_n}
\times{}_{s+2}F_{r+1}\left(\left.\begin{matrix}[n+b_s],n+1+\alpha(1+a)^{-1},\alpha+n(1+a)\\ n+\alpha(1+a)^{-1},[n+c_r]\end{matrix}\right| z\right)L_n^{(an+\alpha)}(x), \tag{8}
$$

which in the particular case $a=0$ reduces to the expansion formula (4) in series of standard (i.e., nonvarying) Laguerre polynomials.

In the right-hand side of Eq. (8), one of the upper parameters of the ${}_{s+2}F_{r+1}$ hypergeometric function is equal to one of the lower parameters plus one. Therefore, taking into account that [17, Vol. II, p. 13]

$$
{}_{p+1}F_{q+1}\left(\left.\begin{matrix}[a_p],c\\ [b_q],d\end{matrix}\right| z\right)=\sum_{n=0}^{\infty}\frac{[a_p]_n(d-c)_n(-z)^n}{[b_q]_n(d)_n n!}\,{}_pF_q\left(\left.\begin{matrix}[n+a_p]\\ [n+b_q]\end{matrix}\right| z\right), \tag{9}
$$

we find the useful alternative expression

$$
{}_{s+2}F_{r+1}\left(\left.\begin{matrix}[n+b_s],n+1+\alpha(1+a)^{-1},\alpha+n(1+a)\\ n+\alpha(1+a)^{-1},[n+c_r]\end{matrix}\right| z\right)
={}_{s+1}F_r\left(\left.\begin{matrix}[n+b_s],\alpha+n(1+a)\\ [n+c_r]\end{matrix}\right| z\right)
+z(1+a)\frac{[n+b_s]}{[n+c_r]}\,{}_{s+1}F_r\left(\left.\begin{matrix}[n+b_s+1],\alpha+n(1+a)+1\\ [n+c_r+1]\end{matrix}\right| z\right). \tag{10}
$$

3.2. Expansion of the exponential function

When the hypergeometric series in the left-hand side does not terminate, Eq. (8) can be considered as a generating function for the varying Laguerre polynomials $\{L_n^{(an+\alpha)}(x)\}$. It is interesting to note that this rather general generating function includes as a particular case the generating function of exponential type derived by Brown [5] and Carlitz [8]. Taking into account that

$$\mathrm{e}^{zx} = {}_0F_0\left(\begin{matrix} - \\ - \end{matrix}\,\middle|\, zx\right),$$

we readily obtain the expansion of the exponential function in series of varying Laguerre polynomials,

$$\mathrm{e}^{zx} = \sum_{n=0}^{\infty} (-z)^n {}_2F_1\left(\begin{matrix} n+\alpha(a+1)^{-1}+1, \alpha+n(1+a) \\ n+\alpha(a+1)^{-1} \end{matrix}\,\middle|\, z\right) L_n^{(an+\alpha)}(x). \tag{11}$$

The hypergeometric function in the right-hand side can be evaluated in exact form by means of Eq. (10) and Newton's binomial theorem, which states that

$${}_1F_0\left(\begin{matrix} b \\ - \end{matrix}\,\middle|\, z\right) = (1-z)^{-b}.$$

Thus we obtain

$$\mathrm{e}^{zx} = (1+az)\sum_{n=0}^{\infty} (-z)^n (1-z)^{-(n(a+1)+\alpha+1)} L_n^{(an+\alpha)}(x), \tag{12}$$

which is equivalent to the exponential generating function given in [5,8].

3.3. Connection formula for varying Laguerre polynomials

When the hypergeometric series in the left-hand side is terminating, Eq. (8) becomes a connection formula giving the expansion of a polynomial in series of the varying Laguerre polynomials $\{L_n^{(an+\alpha)}(x)\}$. For instance, using the hypergeometric representation (3) we find that

$$L_m^{(\beta_m)}(zx) = \frac{(\beta_m+1)_m}{m!}\sum_{n=0}^{m} \frac{(-m)_n(-z)^n}{(\beta_m+1)_n}$$

$$\times {}_3F_2\left(\begin{matrix} n-m, n+1+\alpha(1+a)^{-1}, \alpha+n(1+a) \\ n+\alpha(1+a)^{-1}, n+\beta_m+1 \end{matrix}\,\middle|\, z\right) L_n^{(an+\alpha)}(x), \tag{13}$$

where we have written β_m instead of β to emphasize the fact that the parameters of the Laguerre polynomial in the left-hand side can have an arbitrary dependence on the degree. Using Eq. (10), the ${}_3F_2$ function in the right-hand side can be written as the sum of two ${}_2F_1$ functions,

$${}_3F_2\left(\begin{matrix} n-m, n+1+\alpha(1+a)^{-1}, \alpha+n(1+a) \\ n+\alpha(1+a)^{-1}, n+\beta_m+1 \end{matrix}\,\middle|\, z\right)$$

$$= {}_2F_1\left(\begin{matrix} n-m, \alpha+n(1+a) \\ n+\beta_m+1 \end{matrix}\,\middle|\, z\right)$$

$$+ \frac{(1+a)(n-m)z}{(n+\beta_m+1)}\,{}_2F_1\left(\begin{matrix} n-m+1, \alpha+n(1+a)+1 \\ n+\beta_m+2 \end{matrix}\,\middle|\, z\right),$$

which in the important particular case $z = 1$ can be summed up by means of the Chu–Vandermonde summation formula,

$$ {}_2F_1\left(\begin{matrix} -k, b \\ c \end{matrix} \middle| 1\right) = \frac{(c-b)_k}{(c)_k}. $$

After some algebra, we thus find the connection formula

$$ L_m^{(\beta_m)}(x) = \sum_{n=0}^{m} \frac{(\beta_m - am - \alpha)_{(m-n)(a+1)}}{(m-n)!(\beta_m - am - \alpha + 1)_{(m-n)a}} L_n^{(an+\alpha)}(x), \tag{14} $$

which for $a = 0$ reduces to the known connection formula (5) of the standard (nonvarying) case.

In particular, choosing $\beta_m = bm + \beta$, Eqs. (13) and (14) become connection formulas relating two families of linearly varying Laguerre polynomials. The latter reads,

$$ L_m^{(bm+\beta)}(x) = \sum_{n=0}^{m} \frac{(m(b-a) + \beta - \alpha)_{(m-n)(a+1)}}{(m-n)!(m(b-a) + \beta - \alpha + 1)_{(m-n)a}} L_n^{(an+\alpha)}(x), \tag{15} $$

so that the expression of the coefficients becomes especially simple when either $\alpha = \beta$ or $a = b$. It is also interesting to note that the coefficients only depend on α and β through the difference $\beta - \alpha$, while if $a = b$ they only depend on m and n through the difference $m - n$. Sign properties of the connection coefficients, such as the conditions under which they are nonnegative, can be easily read off from the explicit expressions given in (14) and (15), as done in Ref. [24] for the nonvarying connection formula (5).

4. Applications to molecular potentials

The expansion formulas derived in the previous section are not only compact and elegant, but also useful in the computation of the physical and chemical properties of quantum–mechanical systems. Indeed, for many exactly solvable potentials the solutions of the time-independent Schrödinger equation are controlled by varying classical orthogonal polynomials with arguments that are elementary functions of the coordinate [2]. In particular, varying Laguerre polynomials appear in the eigenfunctions of numerous one-dimensional potentials, such as the Coulomb [16] and Morse [19,21] potentials, which play a relevant role for the theoretical interpretation of ionization phenomena in an intense laser field [26] and the spectroscopic properties of diatomic molecules [21]. In addition, the radial wavefunctions of hydrogenic atoms are also given in terms of varying Laguerre polynomials [2]. The evaluation of the matrix elements of physical observables for these systems naturally requires the expansion coefficients of the associated functions in the varying Laguerre basis, a problem that includes the connection between members of varying Laguerre bases with different parameters.

The lack of an effective quantum–mechanical potential rigorously obtained from first principles has obliged physicists and chemists to use phenomenological potentials with exactly solvable Schrödinger equation to study the properties of molecules, even the diatomic ones. Apart from the harmonic oscillator potential, which provides a good first approximation for the low-lying spectrum of a diatomic molecule, the reference potentials are the Morse potential (which describes reasonably well the high-lying spectrum) and the Pöschl–Teller potential (which describes better some specific degrees of freedom of linear molecules, such as the flexion modes). So, the determination of the physical quantities and electromagnetic transition probabilities of these systems requires the previous knowledge of the connection formula between the wavefunctions of the aforementioned potentials. In the following, we shall use the results of Section 3 to compute the connection formula relating the wavefunctions of two Morse potentials with different parameters (which are controlled by linearly varying Laguerre polynomials), and the connection formula between a Morse wavefunction and a Pöschl–Teller wavefunction (which is controlled by a linearly varying Gegenbauer polynomial).

4.1. Relationship between Morse wavefunctions

The so-called Morse potential is

$$V(x) = V_0\left(\mathrm{e}^{-2\alpha x} - 2\mathrm{e}^{-\alpha x}\right),$$

where V_0 and α are constants. The exact closed form of the normalized eigenfunctions is [19,21]

$$\psi_n(x) = N(n) y^{\lambda-n-1/2}\,\mathrm{e}^{-y/2} L_n^{(2\lambda-2n-1)}(y) \tag{16}$$

for $0 \leqslant n \leqslant [\lambda - \frac{1}{2}]$ (square brackets denote integer part of the expression within), where

$$\lambda = \left(\frac{2\mu V_0}{\hbar^2\alpha^2}\right)^{1/2}, \quad y = 2\lambda \mathrm{e}^{-\alpha x}, \quad N(n) = \left(\frac{\alpha(2\lambda - 2n - 1)n!}{\Gamma(2\lambda - n)}\right)^{1/2}, \tag{17}$$

and μ is the mass of the particle. For the second Morse potential,

$$\tilde{V}(x) = \tilde{V}_0\left(\mathrm{e}^{-2\tilde{\alpha} x} - 2\mathrm{e}^{-\tilde{\alpha} x}\right),$$

the eigenfunctions $\tilde{\psi}_n(x)$ are given by Eqs. (16) and (17) with V_0, α, λ, y, $N(n)$ replaced by $\tilde{V}_0$, $\tilde{\alpha}$, $\tilde{\lambda}$, $\tilde{y}$, $\tilde{N}(n)$, respectively.

For the involved Laguerre polynomials, the connection formula (13) reads

$$L_m^{(2\tilde{\lambda}-2m-1)}(\tilde{y}) = \sum_{n=0}^{m} f_{mn}(x) L_n^{(2\lambda-2n-1)}(y),$$

where

$$f_{mn}(x) = \frac{(n - 2m + 2\tilde{\lambda})_{m-n}}{(m-n)!}\left(\frac{\tilde{y}}{y}\right)^n {}_3F_2\left(\left.\begin{matrix} n-m, n-2\lambda+2, -n+2\lambda-1 \\ n-2\lambda+1, n-2m+2\tilde{\lambda}\end{matrix}\right| \frac{\tilde{y}}{y}\right)$$

and the corresponding relationship for the Morse wavefunctions is

$$\tilde{\psi}_m(x) = \sum_{n=0}^{m} f_{mn}(x) \frac{\tilde{N}(m)}{N(n)} \frac{\tilde{y}^{\,\tilde{\lambda}-m-1/2}}{y^{\lambda-n-1/2}}\,\mathrm{e}^{-(\tilde{y}-y)/2}\psi_n(x). \tag{18}$$

This relation holds provided that $m \leqslant \left[\lambda - \frac{1}{2}\right]$, a condition that is satisfied by the complete set of wavefunctions $\{\tilde{\psi}_m(x)\}$ whenever $\left[\tilde{\lambda} - \frac{1}{2}\right] \leqslant \left[\lambda - \frac{1}{2}\right]$.

4.2. Expansion of Pöschl–Teller wavefunctions in series of Morse wavefunctions

In a similar way, we can write the eigenfunctions of any other one-dimensional potential in terms of the wavefunctions of the Morse potential. Let us consider, for instance, the Pöschl–Teller potential

$$V(x) = -\frac{W_0}{\cosh^2 \kappa x}, \quad W_0 > 0,$$

which is often used as a realistic model for molecular potentials. Its eigenfunctions are essentially varying Gegenbauer polynomials, since their explicit form is [20,21]

$$\phi_n(x) = C_n(1-s^2)^{\beta/2} P_n^{(\beta,\beta)}(s) \tag{19}$$

for $n \leqslant \left[\sqrt{\gamma^2+\frac{1}{4}}-\frac{1}{2}\right]$, where $P_n^{(\alpha,\beta)}(x)$ is the standard Jacobi polynomial,

$$\beta = \beta_n = -n + \sqrt{\gamma^2+\frac{1}{4}}-\frac{1}{2}, \qquad s = \tanh \kappa x, \qquad \gamma^2 = \frac{2\mu W_0}{\hbar^2\kappa^2} \tag{20}$$

and C_n is the normalization constant.

Now we can use Eq. (8) with any of the hypergeometric representations for Gegenbauer polynomials that we can find in the literature. Taking for instance

$$P_m^{(\beta,\beta)}(s) = \frac{(\beta+1)_m}{m!}\, {}_2F_1\left(\begin{matrix} -m, m+2\beta+1 \\ \beta+1 \end{matrix}\,\middle|\, \frac{1-s}{2}\right),$$

we obtain the connection formula

$$P_m^{(\beta,\beta)}(s) = \sum_{n=0}^{m} g_{mn}(x) L_n^{(2\lambda-2n-1)}(y),$$

with

$$g_{mn}(x) = \frac{(m+2\beta+1)_n (n+\beta+1)_{m-n}}{(m-n)!}\left(\frac{1-s}{2y}\right)^n$$
$$\times {}_4F_2\left(\begin{matrix} n-m, n+m+2\beta+1, n-2\lambda+2, -n+2\lambda-1 \\ n+\beta+1, n-2\lambda+1 \end{matrix}\,\middle|\, \frac{1-s}{2y}\right).$$

We thus find the expansion of $\phi_m(x)$ in terms of the Morse eigenfunctions $\psi_n(x)$,

$$\phi_m(x) = C_m(1-s^2)^{\beta/2} \sum_{n=0}^{m} \frac{g_{mn}(x)}{N(n)}\, y^{n+1/2-\lambda}\, e^{y/2} \psi_n(x). \tag{21}$$

Again this relation holds for $m \leqslant \left[\lambda-\frac{1}{2}\right]$, a condition that is satisfied by the complete set of wavefunctions $\{\phi_m(x)\}$ whenever $\left[\sqrt{\gamma^2+\frac{1}{4}}-\frac{1}{2}\right] \leqslant \left[\lambda-\frac{1}{2}\right]$.

5. Summary and open problems

We have shown that a theorem of Verma [31] on generalized hypergeometric functions can be used to determine expansions of arbitrary functions in series of the varying Laguerre polynomials $\{L_n^{(an+\alpha)}(x)\}$. In particular, we have solved the connection problem for these polynomials. The hypergeometric functions approach, previously used to find expansions in series of nonvarying orthogonal polynomials [15,23,25], has thus been shown to be also useful in the varying case.

To illustrate the usefulness of this kind of expansion problems, we have applied them to compute (i) a relationship between the Morse wavefunctions of two molecular states (see Eq. (18)), and (ii) the expansion of a Morse wavefunction describing an arbitrary state of a given molecule in terms of the Pöschl–Teller wavefunctions (see Eq. (21)). These relationships are just two particular cases of a rich variety of expansion problems involving varying classical orthogonal polynomials with nontrivial (at times, even rescaled) arguments, which naturally appear in the computation of the physical quantities and the matrix elements of observables for many-body systems such as atoms, molecules and nuclei. Two open problems of this kind which are relevant in molecular physics for reasons already detailed at the beginning of the previous section are (a) the connection problem between the linearly varying Laguerre polynomials with argument e^{-x} and the rescaled Laguerre polynomials $L_k^{(1)}(2x/k)$, whose solution would enable us to expand Morse wavefunctions in terms of the one-dimensional Coulomb basis, and (b) the expansion problem of the linearly varying Gegenbauer polynomials with argument $\tanh x$ in terms of the linearly varying Laguerre polynomials with argument e^{-x}, whose solution would permit us to expand the Pöschl–Teller wavefunctions in terms of the Morse wavefunctions, i.e., to find the relation inverse to (21).

Acknowledgements

This research was initiated during the visit of the first and second authors to the Instituto Carlos I de Física Teórica y Computacional (Universidad de Granada); both authors wish to acknowledge the hospitality of this institution. This work has been partially supported by the Junta de Andalucía, under the research Grants FQM0207 (J.S.D. and J.S.R.) and FQM0229 (P.L.A.); the Spanish MCyT projects BFM2001-3878-C02 (J.S.R., J.S.D. and P.L.A.) and BFM2000-0206-C04-01 (J.S.R.); and the European Union project INTAS 2000-272 (J.S.D. and J.S.R.).

References

[1] G.E. Andrews, R. Askey, R. Roy, Special Functions, Cambridge University Press, Cambridge, 1999.

[2] V.G. Bagrov, D.M. Gitman, Exact Solutions of Relativistic Wave Equations, Kluwer Academic Publishers, Dordrecht, 1990.

[3] T. Bloom, D.S. Lubinsky, H. Stahl, Interpolatory integration rules and orthogonal polynomials with varying weights, Numer. Algorithms 3 (1992) 55–66.

[4] C. Bosbach, W. Gawronski, Strong asymptotics for Laguerre polynomials with varying weights, J. Comput. Appl. Math. 99 (1998) 77–89.

[5] J.W. Brown, On zero type sets of Laguerre polynomials, Duke Math. J. 35 (1968) 821–823.

[6] V.S. Buyarov, J.S. Dehesa, A. Martínez-Finkelshtein, E.B. Saff, Asymptotics of the information entropy for Jacobi and Laguerre polynomials with varying weights, J. Approx. Theory 99 (1999) 153–166.

[7] B. de la Calle Ysern, G. López Lagomasino, Strong asymptotics of orthogonal polynomials with varying measures and Hermite–Padé approximants, J. Comput. Appl. Math. 99 (1998) 91–103.

[8] L. Carlitz, Some generating functions for Laguerre polynomials, Duke Math. J. 35 (1968) 825–827.

[9] P. Deift, T. Kriecherbauer, K.T.R. McLaughlin, S. Venakides, X. Zhou, Uniform asymptotics for polynomials orthogonal with respect to varying exponential weights and applications to universality questions in random matrix theory, Commun. Pure Appl. Math. 52 (1999) 1335–1425.

[10] J.L. Fields, M.E.H. Ismail, Polynomial expansions, Math. Comp. 29 (1975) 894–902.

[11] J.L. Fields, J. Wimp, Expansions of hypergeometric functions in hypergeometric functions, Math. Comp. 15 (1961) 390–395.

[12] W. Gawronski, B. Shawyer, Strong asymptotics for Jacobi polynomials with varying weights, Meth. Appl. Anal. 6 (1999) 39–54.

[13] E. Grosswald, Bessel Polynomials, Lecture Notes in Mathematics, Vol. 698, Springer, Berlin, 1978, pp. 1–182.

[14] H.L. Krall, O. Frink, A new class of orthogonal polynomials: the Bessel polynomials, Trans. Amer. Math. Soc. 65 (1949) 100–115.
[15] S. Lewanowicz, The hypergeometric functions approach to the connection problem for the classical orthogonal polynomials, preprint, 1998.
[16] R. Loudon, One-dimensional hydrogen atom, Amer. J. Phys. 27 (1959) 649–655.
[17] Y.L. Luke, The Special Functions and their Approximations, Academic Press, New York, 1969.
[18] A. Martínez-Finkelshtein, P. Martínez-González, R. Orive, On asymptotic zero distribution of Laguerre and generalized Bessel polynomials with varying parameters, J. Comput. Appl. Math. 133 (2001) 477–487.
[19] M.N. Nieto, L.M. Simmons Jr., Eigenstates, coherent states and uncertainty products for the Morse oscillator, Phys. Rev. A 19 (1979) 438–444.
[20] A.F. Nikiforov, V.B. Uvarov, Special Functions of Mathematical Physics, Birkhäuser, Basel, 1988.
[21] F. Pérez-Bernal, J.M. Arias, M. Carvajal, J. Gómez-Camacho, Configuration localized wavefunctions: general formalism and applications to vibrational spectroscopy of diatomic molecules, Phys. Rev. A 61 (2000) 042,504.
[22] E.D. Rainville, Special Functions, Macmillan, New York, 1960.
[23] J. Sánchez-Ruiz, Linearization and connection formulae involving squares of Gegenbauer polynomials, Appl. Math. Lett. 14 (2001) 261–267.
[24] J. Sánchez-Ruiz, P.L. Artés, A. Martínez-Finkelshtein, J.S. Dehesa, General linearization formulae for products of continuous hypergeometric-type polynomials, J. Phys. A 32 (1999) 7345–7366.
[25] J. Sánchez-Ruiz, J.S. Dehesa, Some connection and linearization problems for polynomials in and beyond the Askey scheme, J. Comput. Appl. Math. 133 (2001) 579–591.
[26] V. Schwengelbeck, F.H.M. Faysal, Ionization of the one-dimensional Coulomb atom in an intense laser field, Phys. Rev. A 50 (1994) 632–640.
[27] R.L. Shively, On pseudo Laguerre polynomials, Michigan Thesis, 1953.
[28] H.M. Srivastava, Some orthogonal polynomials representing the energy spectral functions for a family of isotropic turbulence fields, Z. Angew. Math. Mech. 64 (1984) 255–257.
[29] N. Temme, Asymptotic estimates for Laguerre polynomials, J. Appl. Math. Phys. 41 (1990) 114–126.
[30] L. Toscano, Funzioni generatrici di particolari polinomi di Laguerre e di altri da essi dipendenti, Boll. Un. Mat. Ital. 7 (3) (1952) 160–167.
[31] A. Verma, A class of expansions of *G*-functions and the Laplace transform, Math. Comp. 19 (1965) 664–666.